ANEJO II

Primera Parte:

Esquema de los procesos metabólicos cinéticos con la formulación y las leyes que rigen cada uno:

Crecimiento

Heterótrofo (Ss) Aeróbico

Nutriente (NH_4^+): 'Aer.GrowthHET(NH4)'

[Energía] + Ss_s Ss +S_{NH4}NH4 + S_{H2O}H2O +S_{HPO4}HPO4 + S_{O2}O2 →S_{XH} XH +S_{HCO3}HCO3 + S_HH

$$r_{aergrowthh\ \ et\ (NH\ 4)} = k_{aergrohet}\ \frac{Ss}{K_{S,het,aer} + Ss}\ \frac{O_2}{K_{O2,het,aer} + O_2}\ \frac{NH_4}{K_{N,het,aer} + NH_4}\ \frac{HPO_4}{K_{HPO\ 4,het,aer} + HPO_4} \cdot X_H$$

Nutriente (NO_3^-): 'Aer.GrowthHET(NO3)'

[Energía] + Ss_s Ss + S_{NO3}NO3 +S_{HPO4}HPO4 +S_{O2}O2 +S_{H2O}H2O → S_{XH}XH + S_{HCO3}HCO3 + S_HH

$$r_{aergrowthh\ \ et\ (NO\ 3)} = k_{aergrohet}\ \frac{Ss}{K_{S,het,aer} + Ss}\ \frac{O_2}{K_{O2,het,aer} + O_2}\ \frac{K_{N,het,aer}}{K_{N,het,aer} + NH_4}\ \frac{NO_3}{K_{N,het,aer} + NO_3}\ \left[\frac{HPO_4}{K_{HPO\ 4,het,aer} + HPO_4}\right] \cdot X_H$$

Heterótrofo (Ss) Anóxico

Oxidante (NO_3^-): 'Anox.GrowthHET(NO3)'

[Energía] + Ss_sSs +S_{NO3}NO3 +S_{H2O}H2O +S_{HPO4}HPO4 → S_{XH}XH +S_{NO2}NO2 +S_{HCO3}HCO3+S_HH

$$r_{anoxgrowth\ \ het\ (NO\ 3)} = k_{anoxgrohet}\ \frac{Ss}{K_{S,het,anox} + Ss}\ \frac{K_{O2,het,aer}}{K_{O2,het,aer} + O2}\ \frac{NO\ 3}{K_{N,het,anox} + NO\ 3}\ \left[\frac{HPO\ 4}{K_{HPO\ 4,het,anox} + HPO\ 4}\right] \cdot X_H$$

Oxidante (NO_2^-): 'Anox.GrowthHET(NO2)'

[Energía] + Ss_s Ss + S_{NO2}NO2 +S_HH → S_{XH}XH +S_{N2}N2 +S_{HPO4}HPO4 +S_{HCO3}HCO3 +S_{H2O}H2O

$$r_{anoxgrowth\ het\ (NO2)} = k_{anoxgrohet} \frac{Ss}{K_{S,het,anox} + Ss} \frac{K_{O2,het,aer}}{K_{O2,het,aer} + O2} \frac{NO2}{K_{NO2,het,anox} + NO2} \left[\frac{HPO4}{K_{HPO4,het,anox} + HPO4}\right] \cdot X_H$$

Autótrofo (Fotosíntesis por algas)

Nutriente (NH_4^+): 'GrowthALG(NH4)'

[Energía] + S_{NH4}NH4 +S_{HPO4}HPO4 +S_{HCO3}HCO3 +S_HH→ S_{XALG}XALG +S_{O2}O2 +S_{H2O}H2O

$$r_{growthalg(NH4)} = k_{groalg} \frac{NO3}{K_{NO3,alg,} + NO3} \frac{NH4}{K_{NH4,alg} + NH4} \frac{HPO4}{K_{HPO4,alg} + HPO4} \cdot \left(\frac{I}{K_I} \exp\left(1 - \frac{I}{K_I}\right)\right) \cdot X_{alg}$$

I, es la radiación solar incidente (W/m2)
$K_{I,}$ es la constante de radiación incidente

Nutriente (NO_3^-): 'GrowthALG(NO3)'

[Energía] + S_{NO3}NO3 +S_{HPO4}HPO4 +S_{HCO3}HCO3 +S_HH +S_{H2O}H2O→ S_{XALG}XALG + S_{O2}O2

$$r_{growthalg(NO3)} = k_{groalg} \frac{NO3}{K_{NO3,alg,} + NO3} \frac{K_{NH4,alg}}{K_{NH4,alg} + NH4} \frac{HPO4}{K_{HPO4,alg} + HPO4} \cdot \left(\frac{I}{K_I} \exp\left(1 - \frac{I}{K_I}\right)\right) \cdot X_{alg}$$

I, es la radiación solar incidente (W/m2)
$K_{I,}$ es la constante de radiación incidente

Consumo

de X_H: 'GrowthCON(XH)'

[Energía] +S_{XH}XH +S_{O2}O2 +S_{H2O}H2O→ S_{NH4}NH4 +S_{HPO4}HPO4 +S_{HCO3}HCO3 +S_{NO2}NO2 +

+ S_HH + S_{XCON} XCON + S_{XS} Xs

$$r_{gro,CON,Xh} = k_{gro,CON} \frac{O2}{K_{O2,CON} + O2} \cdot X_{XH} \cdot X_{CON}$$

de X_S: 'GrowthCON(XS)'

[Energía] +S_{XS} Xs +S_{NO3}NO3 +S_{O2}O2 +S_{H2O}H2O →S_{NH4} NH4 + S_{HPO4}HPO4 +S_{HCO3}HCO3 +

+ S_HH + S_{XCON} XCON

$$r_{gro,CON,Xs} = k_{gro,CON} \frac{O2}{K_{O2,CON} + O2} \cdot X_{Xs} \cdot X_{CON}$$

de X_{N1}: 'GrowthCON(XN1)'

[Energía] +S_{XN1}XN1 +S_{O2}O2 +S_{H2O}H2O→ S_{NH4}NH4 +S_{HPO4}HPO4 +S_{HCO3}HCO3 +S_HH +

+ S_{XCON}XCON + S_{XS} Xs

$$r_{gro,CON,XN1} = k_{gro,CON} \frac{O2}{K_{O2,CON} + O2} \cdot X_{XN1} \cdot X_{CON}$$

de X_{N2}: 'GrowthCON(XN2)'

[Energía] +S_{XN2}XN2 +S_{NO2}NO2 +S_{O2}O2 +S_{H2O}H2O→ S_{NH4}NH4 +S_{HPO4}HPO4 +S_{HCO3}HCO3 +

+ S_{NO3}NO3+ S_HH + S_{XCON} XCON + S_{XS} Xs

$$r_{gro,CON,XN2} = k_{gro,CON} \frac{O2}{K_{O2,CON} + O2} \cdot X_{XN2} \cdot X_{CON}$$

de X_{ALG}: 'GrowthCON(ALG)'

[Energía] + S_{XALG}XALG +S_{NO2}NO2 +S_{O2} O2→ S_{NH4}NH4 + S_{HPO4}HPO4 +S_{HCO3}HCO3 +S_HH +

+ S_{H2O} H2O + S_{XCON} XCON + S_{XI} XI

$$r_{gro,CON,alg} = k_{gro,CON} \frac{O2}{K_{O2,CON} + O2} \cdot X_{alg} \cdot X_{CON}$$

Nitrificación

Reductor (NH_4^+): 'GrowthN1'

[Energía] +S_{NH4}NH4 +S_{HPO4}HPO4 +S_{O2}O2+S_{HCO3}HCO3→S_{XN1}XN1+S_HH+S_{NO2}NO2 +S_{H2O}H2O

$$r_{anoxgrowN1} = k_{anoxgrowN1} \frac{O2}{K_{O2,N1,anox} + O2} \frac{NO3}{K_{NO3,N1,anox} + NO3} \cdot X_{N1}$$

Reductor (NO_2^-): 'GrowthN2'

[Energía] +S_{HPO4}HPO4+S_{O2}O2+S_{HCO3}HCO3+S_HH +S_{NO2}NO2→ S_{XN2}XN2 +S_{NO3}NO3+S_{H2O}H2O

$$r_{anoxgrowN2} = k_{anoxgrowN2} \frac{O2}{K_{O2,N2,anox} + O2} \frac{NO2}{K_{NO2,N2,anox} + NO2} \frac{HPO4}{K_{HPO4,N2,anox} + HPO4} \cdot X_{N2}$$

Respiración

Aerobia

X_H: 'Aer.Resp.HET'

S_{XH}XH +S_{O2} O2 +S_{H2O}H2O→S_{NH4}NH4 +S_{HPO4}HPO4 +S_{XI}XI +S_{HCO3}HCO3 +S_HH +[Energía]

$$r_{aerresphet} = k_{aerresphet} \frac{O2}{K_{O2,het,aer} + O2} \cdot X_H$$

X_{N1}: 'Aer.Resp.N1'

$S_{XN1}XN1 + S_{O2}O2 + S_{H2O}H2O \rightarrow S_{NH4}NH4 + S_{HPO4}HPO4 + S_{XI}XI + S_{HCO3}HCO3 + S_{H}H$ + [Energía]

$$r_{anoxrespN1} = k_{anoxrespN1} \frac{O2}{K_{O2,N1} + O2} \cdot X_{N1}$$

X_{N2}: 'Aer.Resp.N2'

$S_{XN2}XN2 + S_{O2}O2 + S_{H2O}H2O \rightarrow S_{NH4}NH4 + S_{HPO4}HPO4 + S_{XI}XI + S_{HCO3}HCO3 + S_{H}H$ + [Energía]

$$r_{anoxrespN2} = k_{anoxrespN2} \frac{O2}{K_{O2,N2} + O2} \cdot X_{N2}$$

X_{CON}: 'Aer.Resp.CON'

$S_{XCON}XCON + S_{O2}O2 \rightarrow S_{NH4}NH4 + S_{HPO4}HPO4 + S_{HCO3}HCO3 + S_{H}H + S_{XI}XI + S_{H2O}H2O$+[Energía]

$$r_{resp,CON} = k_{resp,CON} \frac{O2}{K_{O2,CON} + O2} \cdot X_{CON}$$

X_{ALG}: 'Aer.Resp.ALG'

$S_{XALG}XALG + S_{O2}O2 \rightarrow S_{NH4}NH4 + S_{HPO4}HPO4 + S_{HCO3}HCO3 + S_{H}H + S_{H2O}H2O$ + [Energía]

$$r_{resp,alg} = k_{resp,alg} \frac{O2}{K_{O2,alg} + O2} \cdot X_{alg}$$

Anóxica

X_H: 'Anox.Resp.HET'

S_{XH}XH +S_{NO3}NO3 +S_HH →S_{NH4} NH4+ S_{N2}N2 +S_{HPO4}HPO4 +S_{XI} XI +S_{HCO3}HCO3 +S_{H2O}H2O +

+ [Energía]

$$r_{anoxresphet} = k_{anoxresphet} \frac{Ss}{K_{S,het,anox} + Ss} \frac{NO3}{K_{N,het,anox} + NO3} \cdot X_H$$

Muerte

X_{ALG}: 'DeathALG' S_{XALG}XALG +S_{NO3}NO3 +S_HH→ S_{NH4}NH4 +S_{HPO4}HPO4 +S_{HCO3}HCO3 +S_{NO2}NO2 +S_{O2}O2 +

+ S_{H2O} H2O + S_{XS} Xs + S_{XI} XI + [Energía]

$$r_{death,alg} = k_{death,alg} \cdot X_{alg}$$

X_{CON}: 'DeathCON' S_{XCON} XCON + S_HH + S_{H2O} H2O → S_{NH4} NH4 + S_{HPO4} HPO4 + S_{HCO3}HCO3 + S_{O2} O2+

+ S_{XS} Xs + S_{XI} XI + [Energía]

$$r_{death,CON} = k_{death,CON} \cdot X_{CON}$$

Hidrólisis

S_{XS} Xs → Ss_s Ss

$$r_{Hid} = k_{Hid} \cdot Xs$$

Segunda Parte:

Los coeficientes estequiométricos obtenidos y modelados en la tesina.

	'SS' moles	'NH4' moles	'NO2' moles	'NO3' moles	'HPO4' moles	'O2' moles	'HCO3' moles	'H' moles	'XH' moles	'XN1' moles	'XN2' moles	'XALG' moles	'XCON' moles	'XS' moles	'XI' moles	'H2O' moles	'N2' moles
Aer. Growth XH(NH4)	-1.67	-0.001			-0.0004	-0.043	0.0358	0.0364	1							-0.014	
Aer. Growth XH(NO3)	-1.67			-0.001	-0.0004	-0.040	0.0358	0.0335	1							-0.020	
Aer. Resp. XH		0.008			0.0009	-0.039	0.0332	0.0268	-1						0.20	-0.018	
Anox. Growth XH(NO3)	-2.00		0.123	-0.123	-0.0003		0.0517	0.0510	1							-0.018	
Anox. Growth XH(NO2)	-3.33		-0.187		0.0001		0.1150	-0.0720	1							-0.018	
Anox. Resp. XH		0.008		-0.031	0.0009		0.0332	-0.0041	-1						0.20	-0.002	
Growth XN1		-0.549	0.541		-0.0010	-0.761	-0.0433	1.0451		1						-0.002	
Aer. Resp. XN1		0.008			0.0009	-0.039	0.0332	0.0268		-1					0.20	-0.014	
Growth XN2			-2.381	2.372	-0.0010	-1.123	-0.0433	-0.0538			1					-0.020	
Aer. Resp. XN2		0.008			0.0009	-0.039	0.0332	0.0268			-1				0.20		
Growth XALG(NH4)		-0.004			-0.0003	0.029	-0.0300	-0.0264				1				-0.006	
Growth XALG(NO3)				-0.004	-0.0003	0.038	-0.0300	-0.0349				1				-0.008	
Aer. Resp. XALG		0.004			0.0003	-0.017	0.0198	0.0165				-1			0.20	-0.014	
Death XALG		0.002			0.0001	0.006	0.0001	-0.0015				-1		0.50	0.12	-0.011	
Growth XCON(XALG)		0.009			0.0006	-0.004	0.0250	0.0177				-5	1	2.00		0.072	0.096
Growth XCON(XS)		0.009			0.0006	-0.139	0.1125	0.1052					1	-3.00		0.002	0.015
Growth XCON(XH)		0.030			0.0039	-0.111	0.0917	0.0694	-5				1	2.00		0.559	
Growth XCON(XN1)		0.030			0.0039	-0.111	0.0917	0.0694		-5			1	2.00		-0.014	
Growth XCON(XN2)		0.030			0.0039	-0.111	0.0917	0.0694			-5		1	2.00		0.009	
Aer. Resp. XCON		0.004			0.0003	-0.017	0.0198	0.0165					-1		0.20	-0.014	
Death XCON		0.002			0.0001	0.006	0.0001	-0.0015					-1	0.50	0.12	0.002	
Hydrolysis	1.00													-1.00		-0.002	